An Integrated Material Characterization-Multiscale Model for the Prediction of Strain to Failure of Heterogeneous Aluminum Alloys

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1 Introduction

An increasing demand for a drastic reduction of energy consumption and for the improvement of engineering systems reliability calls for a significant change of the life assessment models used for design. The traditional way of separating material characterization and structural analysis has to be replaced by a fully integrated method in which the relations between microstructure, structure and damage can be readily investigated. For this, macroscopic fracture needs to be related to the micro-mechanisms of damage in the microstructure. This leads to the need of multiscale modeling so that detailed micro-mechanics analysis can be limited to few critical regions surrounding the cracks. Though a number of multiscale models have been developed for heterogeneous materials over the past decades, they are very often applied to small volumes of material containing only few microscopic features. No real attempt has been made to predict damage behavior of microstructural domain of the size of a laboratory coupon. Such an investigation is highly desirable since the implementation of a design methodology based on multiscale modeling within the industry can be initiated only after a rigorous validation of the method. The present work aims at the development and validation of an *integrated material characterization-multiscale model* for the prediction of

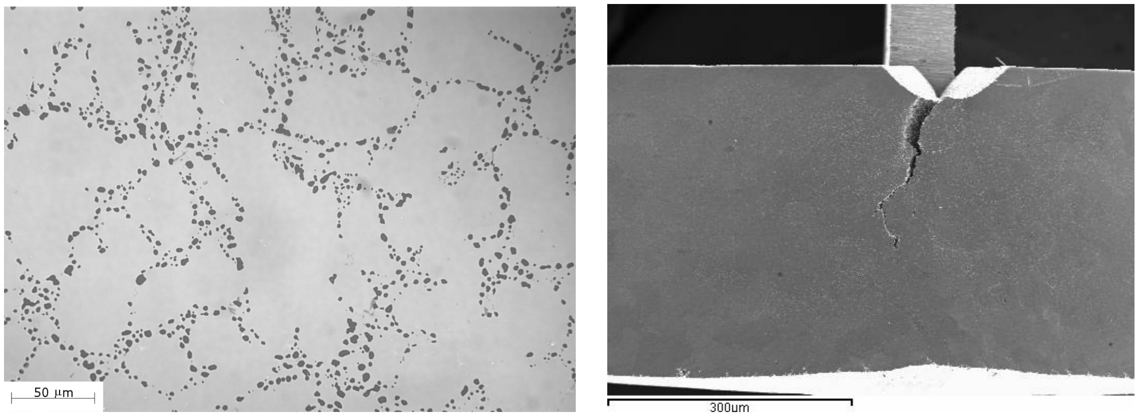
[1]This work would not have been possible without the constant support and advice of my advisor Professor Somnath Ghosh.

strain to failure of heterogeneous aluminum alloys.

Aluminum cast alloys and metal matrix composites are widely used in automotive, aerospace, nuclear and other engineering systems due to their advantageous strength/density ratio. Their microstructure is characterized by a dispersion of hard and brittle heterogeneities in a softer aluminum matrix as depicted in Figure 1(a). The distribution, shape, and size of these heterogeneities affect their failure properties like fracture toughness and ductility in an adverse manner. Important micro-mechanical damage modes that are responsible for deterring the overall properties include particulate fragmentation, debonding at interfaces, and matrix cracking due to void nucleation, growth, and coalescence, culminating in ductile failure as observed in Figure 1(b). To address the needs of a robust methodology for ductility, a comprehensive model for deformation and failure of ductile materials integrating both a material characterization and a multiscale computational model has been developed. The multiscale model used in this work is an extension to ductile fracture of a model originally developed in [1] for microstructurally debonding composites. The present paper is structured as follows. First, the multiscale model for ductile fracture is presented in Section 2. Follows, in Section 3, a description of the material characterization process used as a preprocessor to the multiscale model. This characterization phase is an important step for the incorporation of microstructural features in the numerical model. The capabilities of the integrated material characterization-multiscale model are then demonstrated for a cast aluminum alloy in Section 4.

2 A Concurrent Multiscale Model for Ductile Fracture

In-situ experimental observations of ductile fracture such that of Figure 1(b) reveal that a ductile crack propagates in the microstructure through regions characterized by a high content of inclusions. Ductile fracture is thus controlled by the distribution and morphology of inclusions in vicinity of the crack and an accurate model for strain to failure must include these microstructural features. Unfortunately, a full microscopic description of the entire microstructure is prohibitive



(a) (b)

Figure 1: (a) Micrograph of a A356 cast aluminum alloy, (b) in-situ observation of ductile fracture of a A356 cast aluminum alloy (Micrographs: Courtesy Ford Scientific Research laboratory).

due to the associated computational resources. This leads to the need of multiscale modeling: Micro-mechanisms of damage are simulated in the region surrounding the ductile crack, while a macroscopic description is used for the remaining sub-domain.

An adaptive multiscale model is developed for quantitative predictions at appropriate length scales, following the path of failure from initiation to rupture. Micro-mechanical analysis in regions of dominant damage is performed, while a continuum formulation is used for macroscopic sub-domains. These two length scales of analysis in conjunction with an intermediate swing level form a three-level coupled multiscale model to capture ductile crack propagation in large microstructural domain. The uniqueness of this multiscale framework resides in the explicit modeling of microscopic propagation of damage through a two-way coupling between the micro- and macro-scales. A ”bottom-up” coupling is used to obtain the properties of the macroscopic constitutive relations through homogenization. The additional ”top-down” coupling enables to relate macroscopic failure to the micro-mechanisms of damage through an adaptive propagation of microstructural sub-domains following the microscopic damage, leading to the formation of macroscopic cracks. Hence, no arbitrary homogenization scheme of damage has to be assumed, resulting in very accurate predictions of macroscopic failure.

2.1 Levels in the Concurrent Multiscale Model

The multi-phase material computational domain Ω_{het} is adaptively decomposed into a set of non-intersecting sub-domains, denoted *level-0*, *-1*, *-2*, and *-tr*, i.e. $\Omega_{het} = \Omega_{l0} \cup \Omega_{l1} \cup \Omega_{l2} \cup \Omega_{tr}$. The different levels of computational hierarchy are depicted in Figure 2 and follow the nomenclature adopted in [1]. The concurrent multiscale analysis requires that all levels be coupled for simultaneous solving of variables in the different sub-domains $\Omega_{l0}, \Omega_{l1}, \Omega_{l2}$, and Ω_{tr}. Consequently, the global stiffness matrix and load vectors are derived for the entire computational domain Ω_{het}. The displacement continuity at the boundary between the macroscopic $\Omega_{l0} \cup \Omega_{l1}$ and microscopic $\Omega_{l2} \cup \Omega_{tr}$ sub-domains is satisfied using Lagrange multipliers. The algorithmic treatments corresponding to each level, in order of emergence, are discussed briefly in the following.

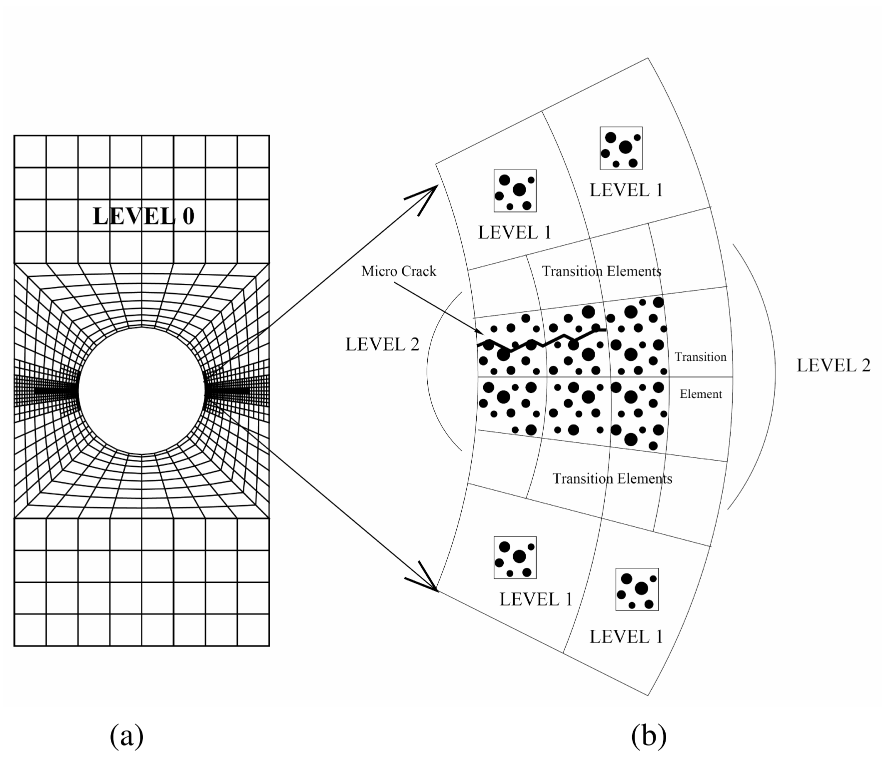


Figure 2: Schematic of a coupled concurrent multi-level model showing: (a) *Level-0* region of macroscopic continuum analysis, (b) blow-up of the critical region surrounding a crack containing *level-1* and *level-2* regions of analysis.

2.1.1 Computational Sub-domain Level-0 (Ω_{l0})

The *level-0* sub-domain corresponds to the region of Ω_{het} for which continuum laws with properties obtained from homogenization are valid in macroscopic analysis. This sub-domain is tessellated into regular Quad-4 elements and is solved using Finite Element (FE) algorithms. Sub-regions of Ω_{l0} may have different microstructure morphology and hence, different plastic and damage properties. The macroscopic constitutive relations used in Ω_{l0} thus need to incorporate the microstructural information related to each of these sub-regions. An Homogenization-based Continuum Plasticity-Damage (HCPD) model [2] for which the parameters are obtained from homogenization of microscopic Representative Volume Elements (RVEs) is developed in the form of an anisotropic Gurson-Tvergaard-Needleman (GTN) model [3]. Calibration of the parameters of the HCPD model is part of the material characterization phase and is further discussed in Section 3.2.

2.1.2 Computational Sub-domain Level-1 (Ω_{l1})

Sub-domain *level-1* is an intermediate computational level for which the HCPD model is valid, but the intensity of the field variables and their gradients indicates an eminent departure from homogeneity. Sub-domain Ω_{l1} is used as a swing region between the macroscopic (Ω_{l0}) and microscopic (Ω_{l2}) sub-domains. The transition of an element e within Ω_{l0} to the intermediate sub-domain Ω_{l1} is determined based on the macroscopic void volume fraction f_e and its gradient through the following criterion:

$$E_e^{gdf} f_e \geq C E_{max}^{gdf} f_{max} \tag{1}$$

where E_e^{gdf} is the norm of the local gradient of void volume fraction f. The quantities f_{max} and E_{max}^{gdf} are the maximum values of all f_e and E_e^{gdf}, and $C \leq 1$ is a prescribed factor.

Two analyzes are required for *level-1* sub-domain. A macroscopic analysis based on the HCPD model (described in Section 3.2) using regular finite element is first performed and the macroscopic fields updated. Then follows a Locally Enhanced Voronoi Cell Finite Element (LE-VCFEM) [4] microscopic analysis of the RVE. The method used to apply the macroscopic strain field e_{ij} on the RVE is described in [2]. The obtained microscopic fields are then used to identify the regions within Ω_{l1} that violate periodicity and thus require a microscopic description.

2.1.3 Computational Sub-domains Level-2 and Level-tr ($\Omega_{l2} \cup \Omega_{tr}$)

Regions of pure microscopic analysis *level-2* emerge from sub-domain Ω_{l1} when periodicity conditions are violated due to localization of the microscopic deformation within the RVE. A macroscopic element e within Ω_{l1} is switched to a microscopic *level-2* description if the following criterion is met:

$$\frac{1}{\int_{\Omega_e} d\Omega} \int_{\Omega_e} H(\varepsilon^p(\mathbf{x}) - \varepsilon^*) d\Omega \geq C \tag{2}$$

where H is the Heaviside step function and $\varepsilon^p(\mathbf{x})$ is the microscopic equivalent plastic strain within the RVE of domain Ω_e. The critical strain ε^* is a threshold for localization and is taken as the macroscopic plastic strain of the RVE at the onset of softening in tension. When the intensity of localization within element e reaches a predetermined value C, the element is switched to the microscopic sub-domain Ω_{l2}.

Discretization of Ω_{l2} is obtained directly from the underlying microstructure as observed in the corresponding micrograph. The microscopic analysis is solved using LE-VCFEM. The computational effort in LE-VCFEM is considerably reduced by the use of a special hybrid FEM formulation that incorporates morphological information of the microstructure [4].

The last level of the multiscale framework is a transitional sub-domain, denoted *level-tr*, used to stabilize the numerical algorithm. It is a microscopic region added at the boundary of Ω_{l2} where the level of damage is very high. The algorithmic treatment of Ω_{tr} is the same as that for *level-2* sub-domain.

3 Material Characterization

To be accurate, the multiscale model for ductile fracture presented in Section 2 must incorporate the effects of microstructural features such as size, shape, orientation, and distribution of inclusions. For this purpose, a two step characterization of the microstructure is introduced as a preprocessor to the multiscale computational model. The first task of the material characterization consists in the identification within the microstructure of the sites prone to damage. These critical regions have to be modeled as microscopic *level-2* sub-domains at the initial stage of the simulation so that damage initiation can be accurately predicted. The second role of the characterization process is the calibration of the material parameters required in the HCPD model of macroscopic sub-domain $\Omega_{l0} \bigcup \Omega_{l1}$. The two steps of the material characterization are described in more details in Sections 3.1 and 3.2 respectively.

3.1 Morphology Based Domain Partitioning

The first step of the material characterization process is to generate the initial multiscale computational domain from a collection of micrographs. The Morphology based Domain Partitioning method (MDP) developed in [5] is used to delineate inhomogeneous sub-domains Ω_{l2} of the microstructure for which a microscopic representation is required and homogeneous sub-domains Ω_{l0} for which a macroscopic representation with periodicity assumption is adequate. If high resolution micrographs are note available for the entire computational domain, a method developed in [5] can be used to reconstruct high resolution microstructural information at all points of the domain from a set of low resolution micrographs and few high resolution micrographs.

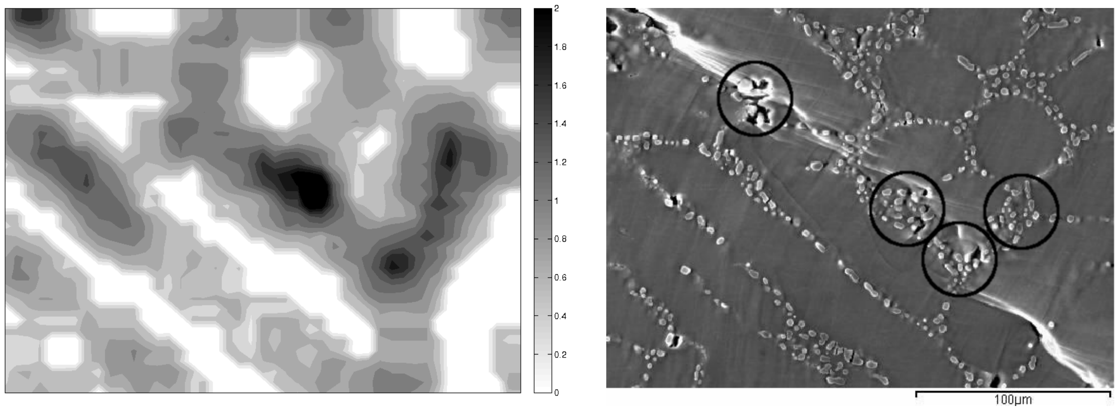
The inhomogeneous sub-domains Ω_{l2} are identified based on their propensity to damage. Propensity to damage is quantified with a metric derived from micro-mechanical simulations. A sensitivity analysis in [6] has shown that strain to failure of heterogeneous alloys is very sensitive to both inclusions morphology and distribution. Large inclusions of high aspect ratios and oriented along the loading axis are ideal sites for damage nucleation. Subsequent damage growth in the matrix and coalescence is controlled by the spatial distribution of inclusions rather than their morphology. As a consequence, microstructures with high levels of clustering have significantly lower strain to failure than those with uniform distributions of inclusions. Based on the sensitivity study in [6], a measure $\tilde{f}$ was proposed in [7] for the identification of the critical regions within a heterogeneous microstructure:

$$\tilde{f} = \frac{\iota}{0.929 - 1.83V_f} \tag{3}$$

This metric is based on the parameters controlling damage growth and coalescence in the matrix, i.e. clustering ι and volume fraction V_f of inclusions. The cluster contour index ι is a measure of clustering developed in [5].

To validate the capability of $\tilde{f}$ to identify the regions prone to damage in a heterogeneous microstructure, the critical regions predicted by equation (3) have been compared to experimental observations made at Ford Scientific Research Laboratory (FSRL) in [7]. The results of this validation are reported in Figure 3. The microstructural domain considered has horizontal and vertical dimensions of 147 μm x 125 μm and the corresponding contour plot of $\tilde{f}$ is plotted in Figure 3(a). Four regions are identified as critical in the microstructure, corresponding to the darker regions. The experimental observation made during a microscopic bending test at FSRL is shown at Figure 3(b). The micrograph shows that damage, at the onset of strain localization and final failure, is mainly located in three of the four predicted regions. This confirms that $\tilde{f}$ is an effective parameter for the determination of the critical regions within a microstructural domain of an aluminum cast alloy.

The microscopic sub-domains are identified through a domain partitioning algorithm based on the morphological descriptor $\tilde{f}$ indicating weak regions in the microstructure. This algorithm delineates the initial microscopic sub-domains based on a statistical analysis of $\tilde{f}$ within the microstructure similar to that developed in [5]. The regions that are statistically non-homogeneous are



(a) (b)

Figure 3: (a) Contour plot of $\tilde{f}$ for the microstructure of Figure 3(b), (b) in-situ observation of ductile fracture of a A356 cast aluminum alloy: Cracked particles at the onset of localization of damage (Micrograph: Courtesy Ford Scientific Research Laboratory).

represented as pure microscopic elements in the multiscale analysis. Once the non-homogeneous regions Ω_{l2} are identified, all the homogeneous sub-domains are merged to form a macroscopic sub-domain Ω_{l0}. This results in an initial mesh for the multiscale simulation as illustrated in Figure 5(a) where three critical regions were identified. The microstructure of one of these regions is shown in Figure 5(c).

3.2 Homogenized Model for Heterogeneous Materials

The second step of the material characterization is the development of macroscopic constitutive relations for macroscopic sub-domain $\Omega_{l0} \bigcup \Omega_{l1}$ that incorporate the microstructural features. Effective constitutive relations are obtained by averaging the mechanical response of a RVE with imposed periodicity boundary conditions. Macroscopic analysis with the effective constitutive model reduces significantly the computational effort in comparison with a complete microscopic analysis. A methodology for the determination of regions of the initial sub-domain Ω_{l0} requiring different set of macroscopic properties has been developed in [5]. Once the RVE of each region of Ω_{l0} has been identified using the statistical analysis described in [2], the parameters of the

Homogenization-based Continuum Plasticity-Damage (HCPD) model are calibrated using asymptotic homogenization.

The HCPD model is a modification of the GTN model [3] that captures the strong anisotropy resulting from the non-homogeneous distribution of inclusions and the associated constrained plastic flow. The novelty of the HCPD model is the introduction of anisotropic parameters that evolve with plastic deformation and damage. Effects of load history are accounted for through the projection of the flow rule on an evolving principal material coordinate system. The anisotropic yield function is expressed in the principal coordinate system in terms of the deviatoric and hydrostatic components of the macroscopic stress tensor, denoted Σ_{eq} and Σ^{hyd}, and the void volume fraction f as:

$$\bar{\Phi} = \frac{\Sigma_{eq}^2}{Y_f^2(W_p)} + 2Q_1 f \cosh\left(\frac{3Q_2}{2}\frac{\Sigma^{hyd}}{Y_f(W_p)}\right) - 1 - (Q_1 f)^2 = 0 \tag{4}$$

where Y_f is the flow stress of the unvoided matrix and is a function of the plastic work W_p. Σ_{eq} is Hill's equivalent stress for which the anisotropic parameters are calibrated from asymptotic homogenization and evolve with increasing plastic flow:

$$\Sigma_{eq}^2 = F(W_p)(\Sigma_{yy} - \Sigma_{zz})^2 + G(W_p)(\Sigma_{zz} - \Sigma_{xx})^2 + H(W_p)(\Sigma_{xx} - \Sigma_{yy})^2 + C(W_p)\Sigma_{xy}^2 \tag{5}$$

Parameters Q_1 and Q_2 in equation (4) are associated with the hydrostatic stress and are also calibrated from homogenization. Another particularity of the HCDP model is a novel damage nucleation criterion developed from homogenization of data on inclusion fragmentation in the RVEs. The details of the strain controlled nucleation model may be found in [2].

Figure 4 shows the capability of the HCPD model to capture ductile mechanisms of deformation and damage for highly anisotropic heterogeneous materials. A very good agreement is found between the predicted stress-strain behavior using the HCPD model and the corresponding micromechanics simulation for different loading conditions. This homogenization based macroscopic model is used in the multiscale computational model for the macroscopic sub-domain $\Omega_{l0} \bigcup \Omega_{l1}$.

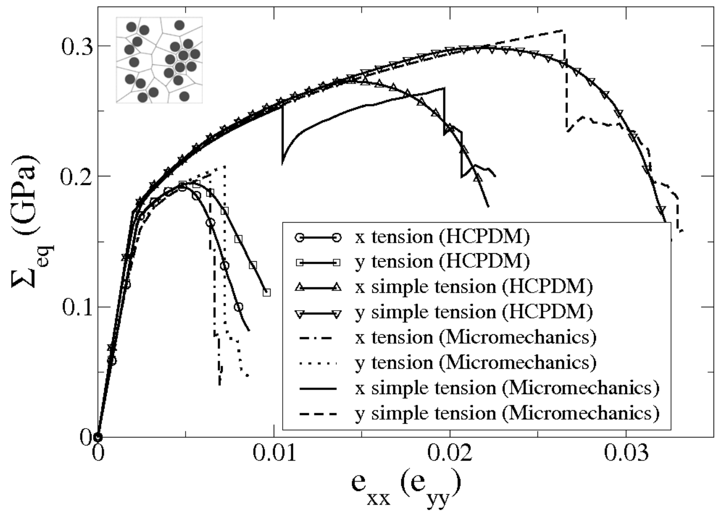


Figure 4: Equivalent stress-strain plot under different loading conditions comparing the HCPD model to micro-mechanics simulations.

4 Numerical Example

The ability of the integrated material characterization-multiscale model for ductile fracture is demonstrated in this section for a cast aluminum alloy W319. A rectangular microstructural domain of dimensions 384 μm x 1536 μm is loaded in uniaxial tension in the vertical direction. The characterization of the microstructure using the morphology based domain partitioning method (MDP) described in Section 3.1 leads to the identification of three inhomogeneous regions that need to be modeled as microscopic *level-2* at the initial stage of the simulation. The homogeneous regions are then merged to form a homogenized *level-0* sub-domain leading to the initial partitioning depicted in Figure 5(a). The microstructure of one of the three critical regions is shown in Figure 5(c).

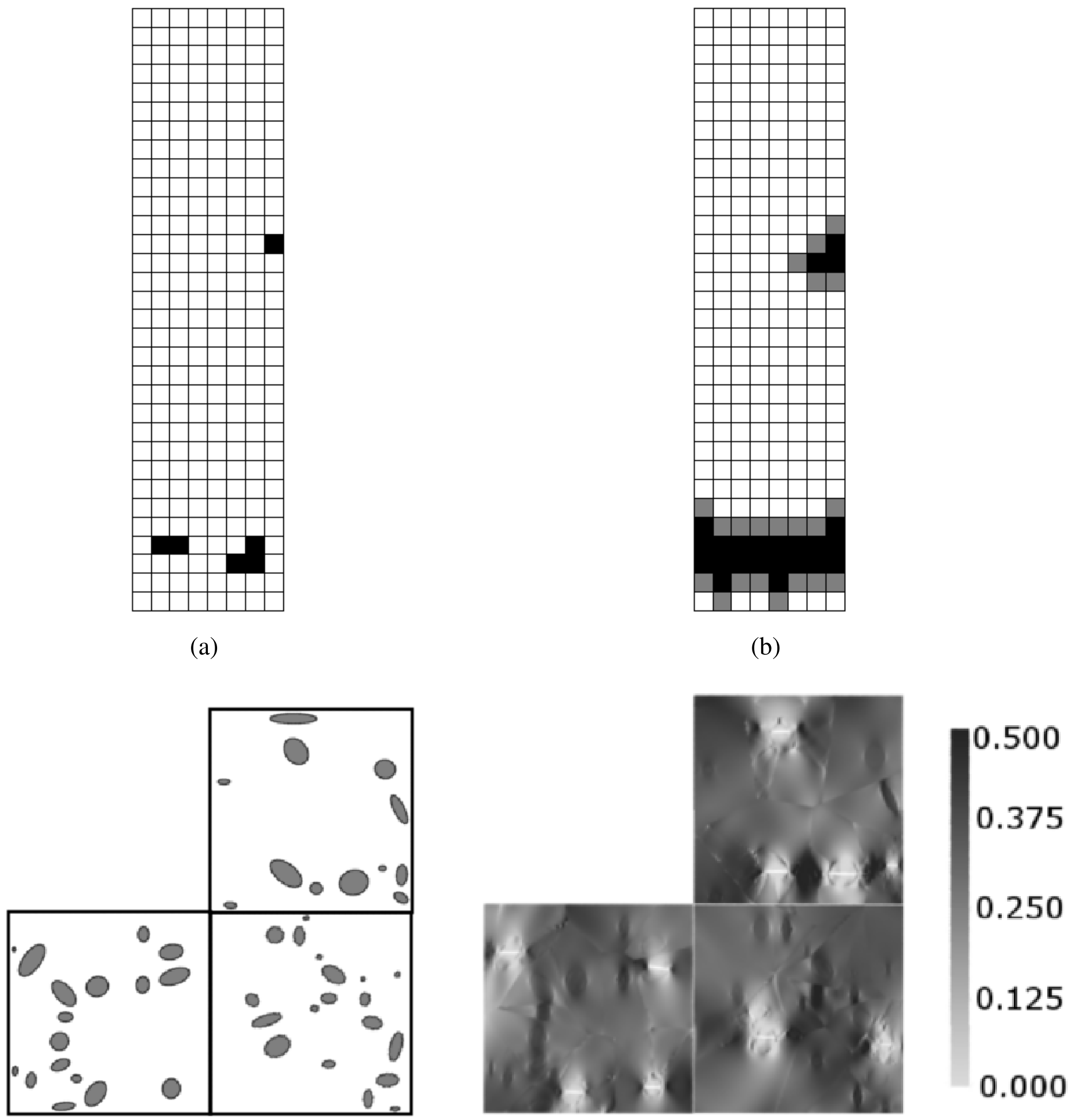
During the simulation, adaptivity and level transition lead to the propagation of sub-domain Ω_{l2} perpendicularly to the applied load. Consequently, the surrounding Ω_{l0} elements are switched to Ω_{l1} due to the high gradients induced by the propagation of damage. This process results in the formation of macroscopic cracks and ultimately in final fracture. Figure 5(b) shows the spatial distribution of the different levels of the multiscale model once the coalescence of the cracks emerging from two of the critical regions have led to the formation of a macroscopic crack. A contour plot of microscopic stress within the microstructure of Figure 5(c) is shown in Figure 5(d). Ductile fracture mechanisms of damage nucleation, growth, and coalescence are very well captured by the proposed multiscale model.

5 Conclusion

A new model for ductile fracture of heterogeneous materials has been presented in this paper. This concurrent and adaptive multiscale model successfully captures the micro-mechanisms of ductile fracture through a two-way coupling between the micro- and macro-scales. Micro-mechanical analysis is performed for the critical region surrounding a crack, while the remaining of the domain is modeled as a continuum medium. These two length scales in conjunction with an intermediate swing level form a three-level coupled multiscale model. Evolution of damage in the microstructure results in the propagation of microscopic sub-domains that leads to the formation of macro-cracks. The incorporation of microstructural information in the model is assured by a material characterization used as a preprocessor to the multiscale model. During that phase, the initial microscopic and macroscopic sub-domains Ω_{l2} and Ω_{l0} are first delineated. Then, the properties of the macroscopic regions are obtained from asymptotic homogenization of RVEs.

The capabilities of the model have been successfully demonstrated on a cast aluminum alloy W319 for moderate microstructural domain. The need for rigorous validation of the model with experiments requires simulations of the length scale of laboratory specimens. The numerical implementation of the model is currently extended to simulations of that scale.

An immediate benefit of the multiscale model presented in this work is in the prediction of strain to failure of simulated microstructures obtained from casting simulations at FSRL. The pro-



(c) (d)

Figure 5: Spatial distribution of *level-2* (black), *level-1* (gray) and *level-0* (white) elements (a) at the beginning of the simulation and (b) after coalescence of the macroscopic cracks, (c) microstructure of one of the critical regions, (d) contour plot of the microscopic vertical normal stress within the region shown in (c) (GPa).

posed model can also be used to address new classes of problems that have never been investigated before. An example is the analysis of synergistic or competitive influences of microstructure morphology and structural geometry on ductile fracture of structural components. It would also be of great practical interest to extend the present deterministic model to stochastic predictions of strain to failure based on the variability of the microstructure.

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